PRACE and the HPC Tiers

Per Öster

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CSC – Tieteen tietotekniikan keskus Oy
CSC – IT Center for Science Ltd.

- Intro CSC
- General overview of PRACE
- PRACE Tiers
- Role of Tier-1 and opportunity for non-hosting partners

CSC -
IT Center for Science

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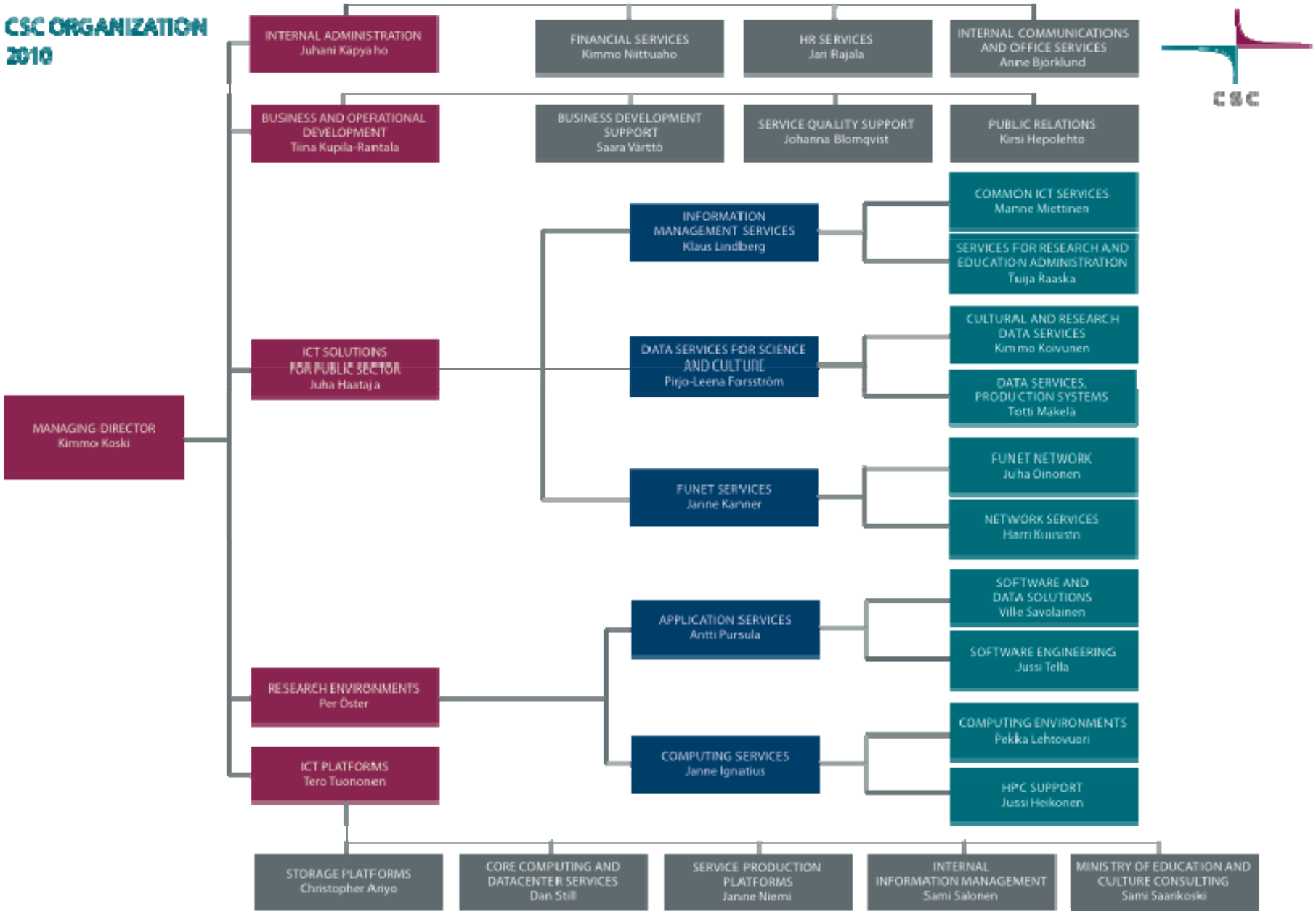
CSC – IT Center for Science Ltd.

CSC at a glance

- Founded in 1971 as a technical support unit for Univac 1108
- Connected Finland to the Internet in 1988
- Reorganized as a company, CSC – Scientific Computing Ltd. in 1993
- All shares to the Ministry of Education of Finland in 1997
- Operates on a non-profit principle
- Facilities in Espoo, close to Otaniemi campus (of 15,000 students and 16,000 technology professionals)
- Staff >190
- Turnover 2009 21,8 million euros

CSC ORGANIZATION 2010



Mission

- CSC, as part of the Finnish national research structure, develops and offers high-quality information technology services

Customers

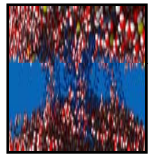
- 3000 researchers use CSC's computing capacity
- Funet connects about 80 organizations to the global research networking infrastructure
  - universities
  - polytechnics
  - 35 industrial clients and research institutions
  - Total of 350 000 end users

Research Environments Business Area

Computing Services

- Computing Environments
- HPC Support

Application Services



- Software and Data Solutions
- Software Engineering

CSC's CrayXT4/XT5

CRAY XT4/XT5 alias Louhi

- 2356 AMD Quad Opteron 2,3 GHz CPUs
- 10864 cores
- Memory ~ 11,7 TB
- Theoretical computing power 100 teraflop/s

Computing servers

Louhi: CRAY XT4/XT5

- 2716 x 4 AMD 2,3/2.6 GHz = 10864 cores
- 8/4 GB memory / node
- > 100 Teraflop/s
- Profile: Parallel processing

Hippu: HP ProLiant DL785 G5

- 2 x 32 AMD 2.5 GHz = 64 cores
- 0.5TB memory / node
- Profile: Interactive use, large memory, plenty of applications

Murska: HP-CP4000BL ProLiant supercluster

- 544 x 2 x 2 AMD 2.6 GHz = 2178 cores
- 32/16/8/2 GB memory / node
- Interconnect: Infiniband
- Profile: Broad software selection

Vuori: HP CP4000 BL Proliant supercluster

- 240 x 2 x 12 AMD 2.6 GHz = 2880 cores
- 32/16 GB memory/ node
- Interconnect: Infiniband
- Profile: broad software selection

Grid infrastructures and projects in Finland

- Grid makes it possible to:

  combine, distribute and administer resources such as computers, storage, network connections, scientific instruments and application services across organizational boundaries.

M-grid

Distributed European Infrastructure for Supercomputing Applications

EGI

NDGF
Nordic DataGrid Facility

MBRACE Grid
Network of excellence

LCG

gLite

UNICORE

NORDUGRID
Grid Solution for Wide Area Computing and Data Handling

the globus toolkit

Computing Services
Basic services/support

- Porting
  - From compiler support to code modification and, in special cases, even rewriting (e.g. from Matlab or R to Fortran)
  - GPGPU porting in the FinnovativeComputing project
- Parallelization
  - From templates to full codes
  - I/O parallelization
  - MPI/OpenMP hybridization
- Optimization
  - Support for performance analysis tools (profilers etc.)
  - Compiler flags (with CSC developed OpFla tool)
  - Advanced optimization requiring code modification
  - Recommending/changing algorithms

Application Services

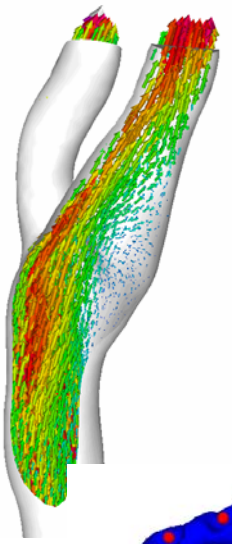
Basic Services and support

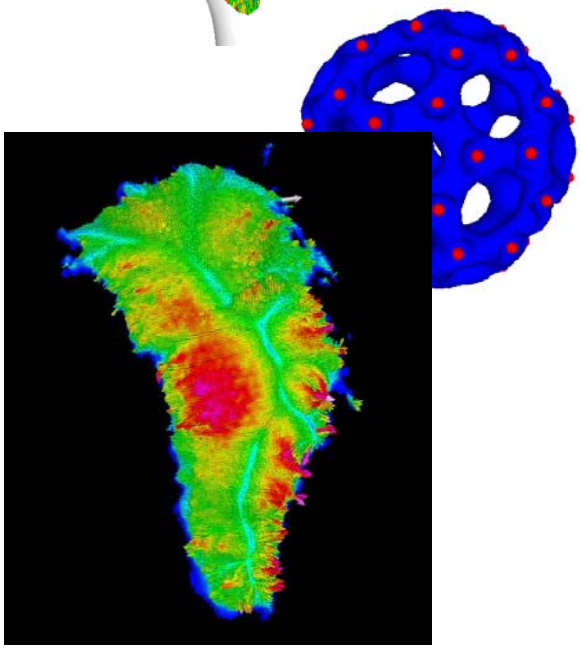
- Wide collection of scientific software
- Consultancy, training and support on scientific software and computational science
- Coordination of national software consortia
- Participation in EU projects such as HPC-Europa2, EMBRACE and ELIXIR (ESFRI)
- Software development and maintenance

Application Services

Software Engineering

- ELMER
  - Finite element package for multi-physics problems
  - Collaboration since more that 10 years between CSC, Finnish Universities and industry



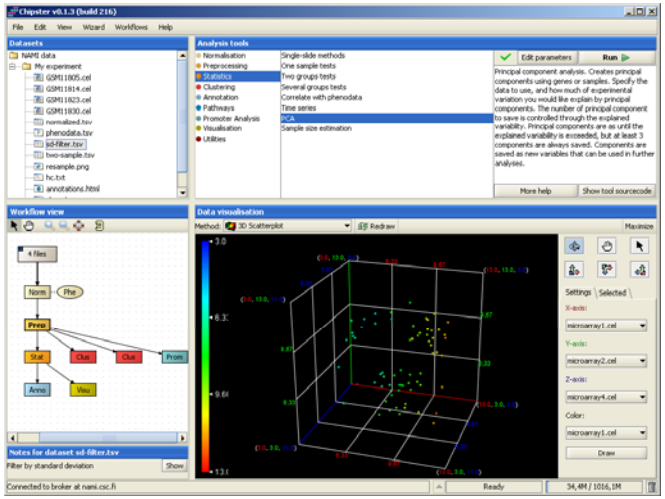


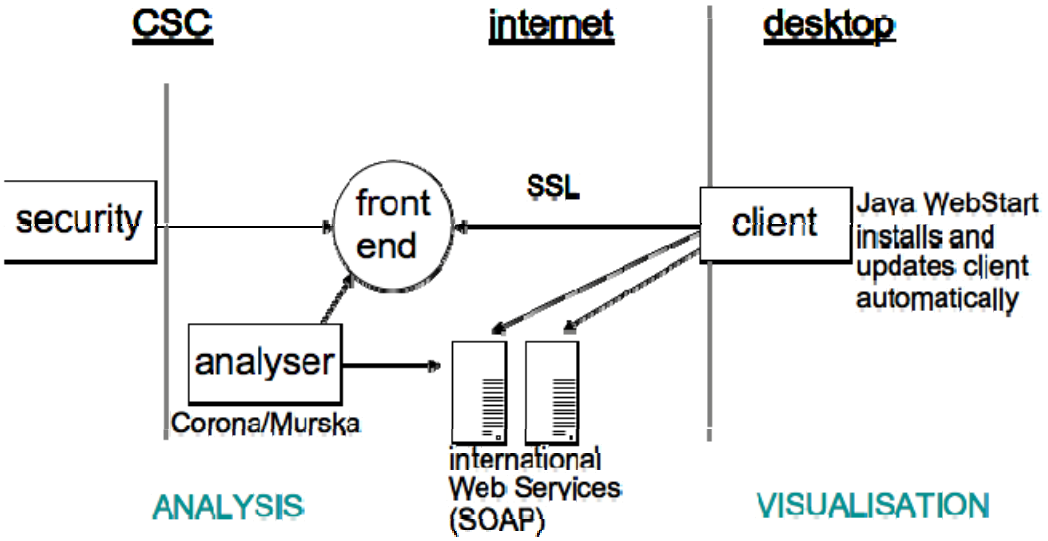
http://www.csc.fi/elmer

Application Development

Software Engineering

- Chipster - Platform for Data Analysis
  http://chipster.csc.fi
  - DNA Micro-array data analysis
  - Enables researcher to create a workflow combining remote compute resources and web-services with built-in or own developed analysis algorithms
  - Open source development by CSC with user input from the Finnish bioscience community





HPCE2 visitor program

- 7 computing centers participating
  - Finland, France, Germany, Italy, Netherlands, Spain, UK
  - These countries are eligible for hosting visits
- Funding for research visits includes
  - travel costs
  - daily allowance
  - accommodation costs
  - access to computing facilities
- Visit length 2 – 13 weeks

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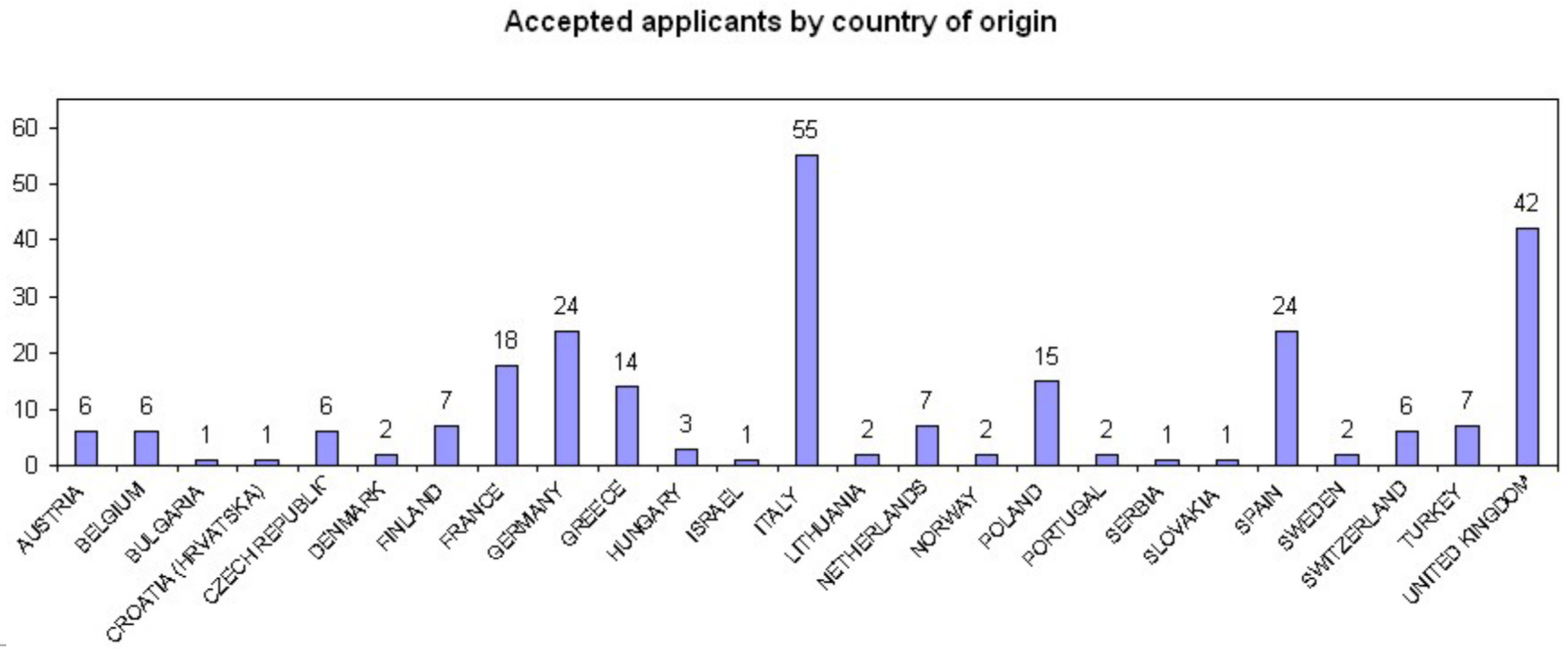
Statistics

- Acceptance rate in 2009: 75%
- Total number of visitors in 2009: 255



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PRACE – Building a new e-infrastructure in Europe

HellasHPC – 22 October 2010

Per Öster

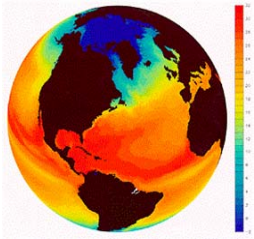
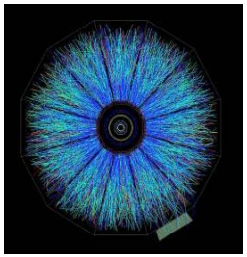
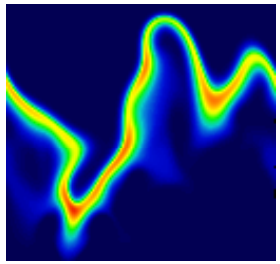
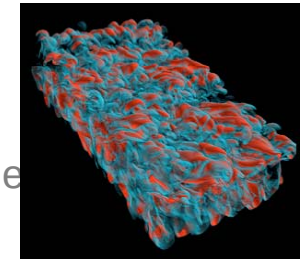
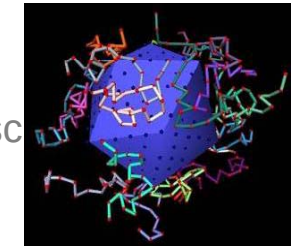
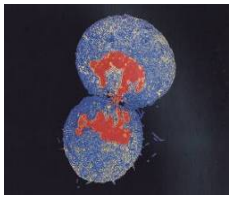
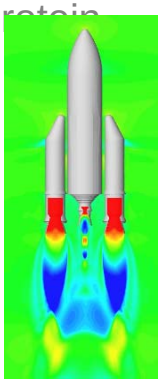
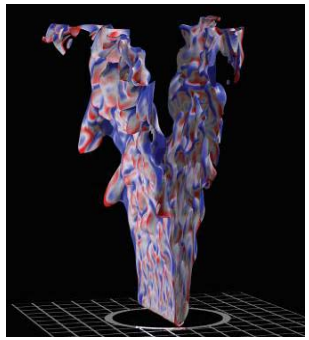
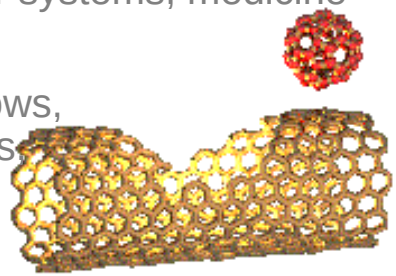
CAPACITIES

e-infrastructure

PRACE
The Partnership for Advance Computing in Europe is ***the*** European HPC Research Infrastructure

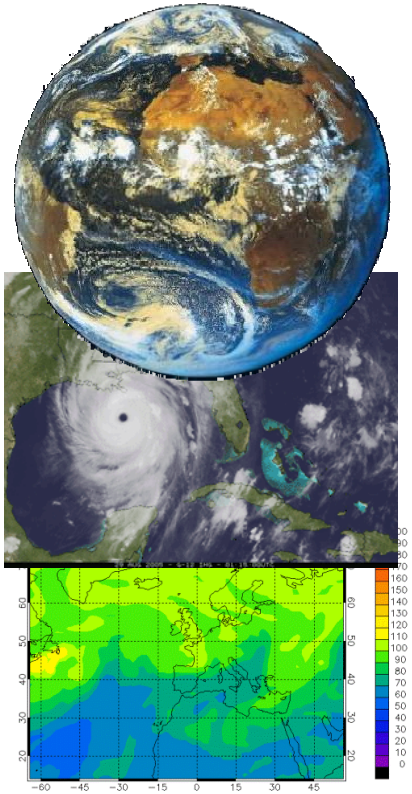
- PRACE enables world-class science through large scale simulations
- PRACE provides HPC services on leading edge capability systems on a diverse set of architectures
- PRACE operates up to six Tier-0 systems as a single entity including user and application support
- PRACE offers its resources through a single pan-European peer review process
- PRACE is providing services since August 2010
- The first Tier-0 system is the fastest Supercomputer in Europe

Why?

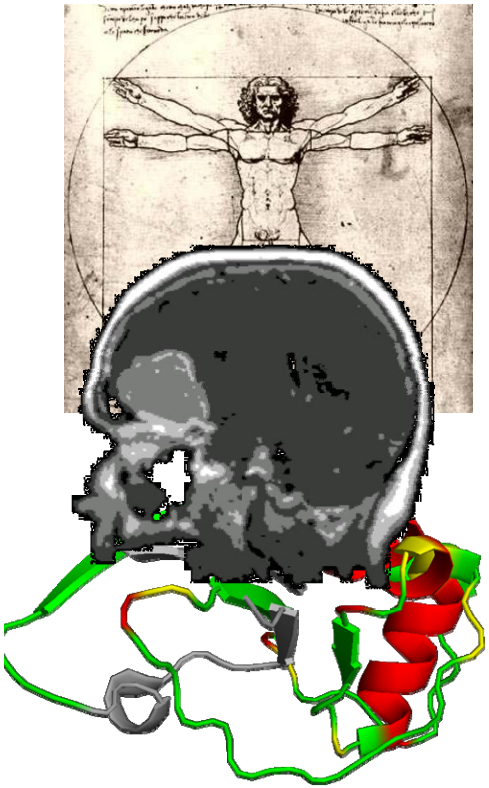










- Weather, Climatology, Earth Science
  - degree of warming, scenarios for our future climate.
  - understand and predict ocean properties and variations
  - weather and flood events
- Astrophysics, Elementary particle physics, Plasma physics
  - systems, structures which span a large range of different length and time scale
  - quantum field theories like QCD, ITER
- Material Science, Chemistry, Nanoscience
  - understanding complex materials, complex chemistry, nanosc
  - the determination of electronic and transport properties
- Life Science
  - system biology, chromatin dynamics, large scale protein dynamics, protein association and aggregation, supramolecular systems, medicine
- Engineering
  - complex helicopter simulation, biomedical flows, gas turbines and internal combustion engines, forest fires, green aircraft,
  - virtual power plant

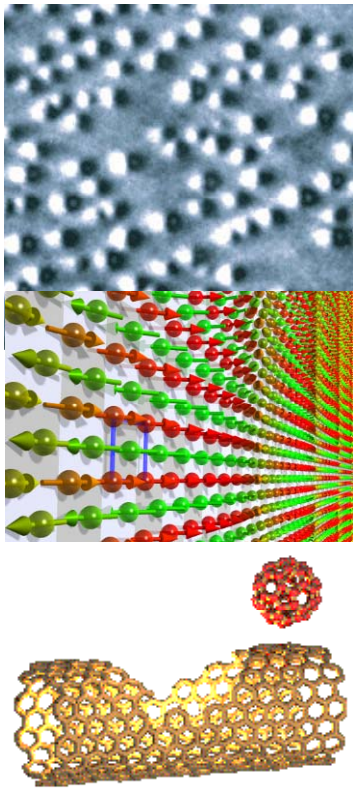
Supercomputing Drives Science through Simulation



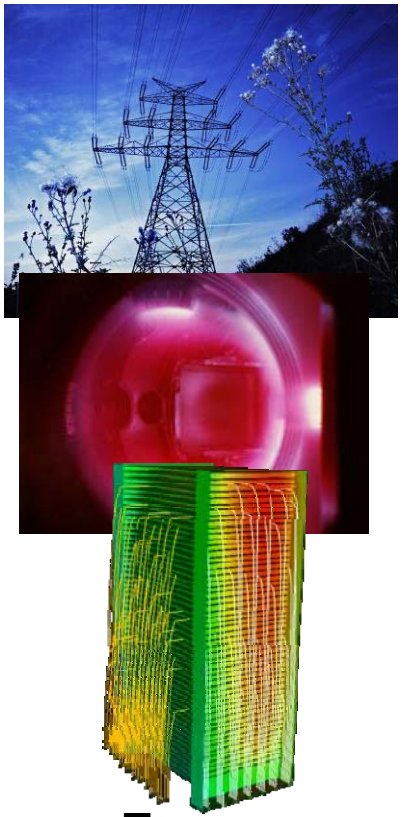
Environment
Weather/ Climatology
Pollution / Ozone Hole



Ageing Society
Medicine
Biology



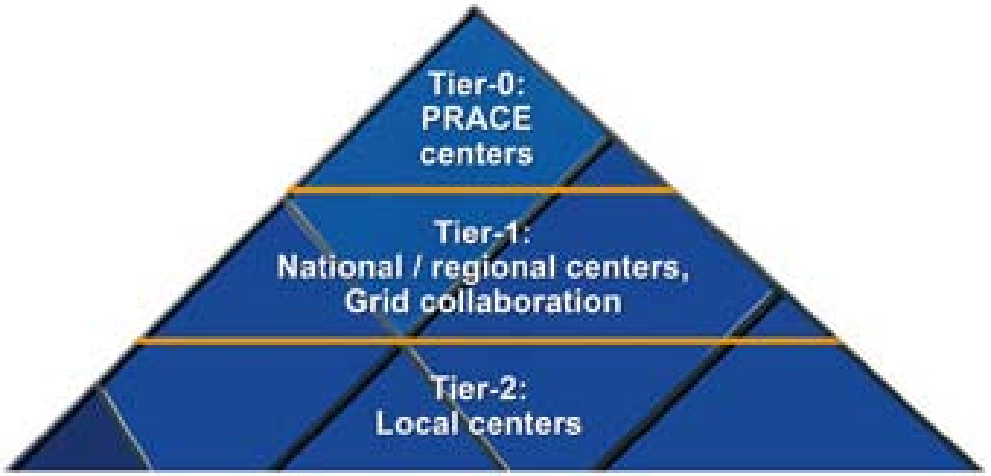
Materials/ Inf. Tech
Spintronics
Nano-science



Energy
Plasma Physics
Fuel Cells

The European HPC Ecosystem

- PRACE prepares the creation of a persistent pan-European HPC service, consisting of several tier-0 centres providing European researchers with access to capability computers and forming the top level of the European HPC ecosystem.
- PRACE is a project funded in part by the EU's 7th Framework Programme.



First Milestone: HPC in ESFRI Roadmap

The European Roadmap for Research Infrastructures is the first comprehensive definition at the European level

Research Infrastructures are one of the crucial pillars of the European Research Area

A European HPC service – impact foreseen:

- strategic competitiveness
- attractiveness for researchers
- supporting industrial development

Second Milestone

- Memorandum of Understanding signed by 15 States in Berlin, on April 16, 2007

- France, Germany, Spain, The Netherlands, UK and Italy committed funding for a European HPC Research Infrastructure

Third Milestone: The PRACE Project

EU approved the PRACE Preparatory Phase Project **(Grant: INFSO-RI-211528)**

- 16 Partners from 14 countries
- Project duration:
  January 2008 –June 2010
- Project budget: 20 M € ,
  EC funding: 10 M €
- Kickoff: Jülich, January 29-30, 2008

CAPACITIES

e-infrastructure

Fourth Milestone: PRACE RI created

- The PRACE Research Infrastructure was created on April 23, 2010 in Brussels

Fifth Milestone: PRACE Inauguration

- Four nations (France, Germany, Italy and Spain) have agreed to provide 400 million Euro to implement supercomputers with a combined computing power in the multi Petaflop/s range over the next 5 years.
- This funding is complemented by up to 70 million Euros from the European Commission which is supporting the preparation and implementation of this infrastructure.

Sixth Milestone: PRACE project completed

- In October 2009 PRACE demonstrated to a panel of external experts and the European Commission that the project made “satisfactory progress in all areas” and “that PRACE has the potential to have real impact on the future of European HPC, and the quality and outcome of European research that depends on HPC services”. Two months before the end of the project it met the eligibility to apply for a grant of 20 million Euros for the implementation phase of the permanent PRACE Research Infrastructure.
- The First Implementation Project (PRACE 1IP) started on July 1, 2010

PRACE Project Achievements in a Nutshell

- Prepared the Creation of the permanent pan-European Research Infrastructure as a legal entity
- Established the PRACE brand
- Provided extensive HPC Training
- Deployed and evaluated promising Architectures
- Ported and petascaled applications

Installed prototypes

IBM BlueGene/P (FZJ)
01-2008

IBM Power6 (SARA)
07-2008

Cray XT5 (CSC/CSCS)
11-2008

IBM Cell/Power
(BSC)
12-2008

NEC SX9, vector part (HLRS)
02-2009

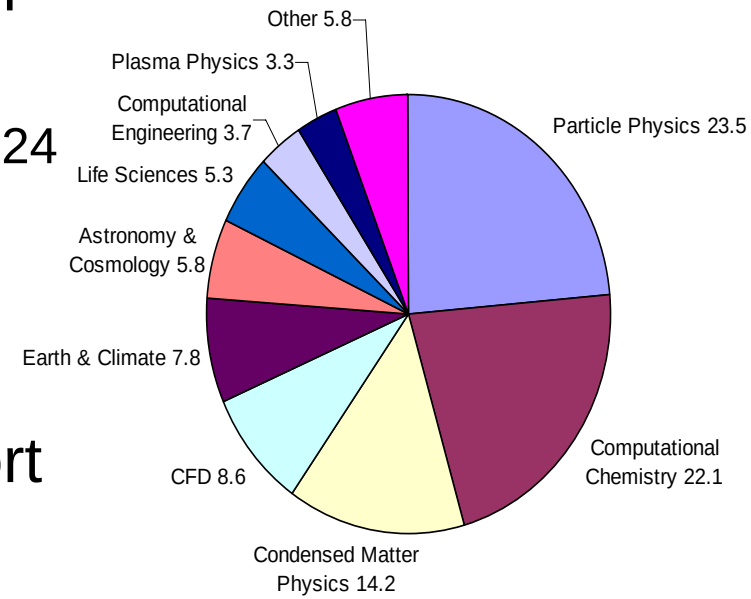
Intel Nehalem/Xeon (CEA/FZJ):
06-2009

23 scientific software ported and tested to prototype-systems

- The applications studied in this work cover a broad range of scientific areas, and are representative of the European HPC usage. Most of them also originate from the European scientific community.
- The applications are: Alya, AVBP, BSIT, Code_Saturn, CP2K, CPMD, Echam5, Elmer, EUTERPE, Gadget, GPAW, Gromacs, HELIUM, NAMD, NEMO, NS3D, Octopus, PEPC, SIESTA, SPECFEM3D, QCD, Quantum_Espresso and WRF.
- These applications were ported, evaluated and scaled on the PRACE prototypes, which represent the current top of the line supercomputer architectures.
- The applications were ported, on average, to three prototype systems.

Categorisation of Applications

- Benchmark applications should be *representative* of European HPC usage
- We conducted surveys of PRACE partners' HPC systems and major applications
  - Collecting various interesting data for 24 systems and 69 applications
- Quantitative basis for selecting representative applications
- Disseminated as Technical Report



Future technologies and STRATOS: PRACE Advisory group for Strategic Technologies,

- Exascale Software
- Technology Watch
- Green-IT and HPC Leadership resources
- Many HPC stakeholders and enterprises have expressed their interest in becoming part of STRATOS.
- 9 prototypes representing promising future HPC technologies, such as computational accelerators, have been deployed and are being evaluated.
- Key results published in March 2009

Applications: Petascaling and Optimisation

Petascaling

- Mixed-mode parallelisation
- Load balancing
- Minimisation of communication overheads
- Parallel I/O
- Checkpointing

Optimisation

- Optimising serial performance
  - CPU
  - Memory
- Optimising both for general-purpose architectures and specialised architectures
- Algorithmic optimisations

PRACE will disseminate
best practice *in these areas*

Libraries and Programming Models

- Classification of Benchmark applications
- Current programming models
  - MPI, OpenMP, mixed-mode, …
- PGAS and other future programming models
- Accelerator Languages
  - CUDA, RapidMind, openCL …
- Petascale libraries

Survey of HPC education and training needs

- The Top 10 users at each participating PRACE member site were invited to participate in completing the survey.
- The data was obtained from the most comprehensive evaluation of user training requirements
- Over 90%) of respondents believed they would benefit from formal training in the following areas: performance optimization, debugging tools and techniques, code testing and compiler optimisations;
- Over 90% of users considered that there is an important need for improved HPC training programmes

Training: Benchmarking the survey

- After publication of the PRACE HPC Training and Education survey, a request was received from the Hong Kong Institute of High Performance Computing to use the survey as a template for a similar survey in North-East Asia (http://survey2008.hkhpc.org/).

- Recently a further request was received from U.S. TeraGrid trainers to use the survey as a basis for their latest TeraGrid educational and training survey."

Current status

- 20 European countries are currently part of PRACE
- 4 hosting partners
- The PRACE project implementation phase started on July 1. 2010

PRACE Implementation Phase Work Packages

- WP1 Management
- WP2 Evolution of the Research Infrastructure
- WP3 Dissemination and training
- WP4 HPC Ecosystem Relations
- WP5 Industrial User Relations
- WP6 Technical Operation and Evolution of the Distributed Infrastructure
- WP7 Enabling Petascale Applications: Efficient Use of Tier-0 Systems
- WP8 Support for the procurement and commissioning of HPC services
- WP9 Future Technologies

Accessing the PRACE RI

Access Model

- Based on peer-review: “the best systems for the best science”
- Three types of resource allocations
  - Test / evaluation access
  - Project access – for a specific project, grant period ~ 1 year
  - Programme access – resources managed by a community
- Free-of-charge

Funding

- Mainly national funding through partner countries
- European contribution
- Access model has to respect national interests (ROI)

Access for the systems

http://www.prace-project.eu/hpc-access

Future integration into the HPC ecosystem

- Software builds on the developments in the DEISA project
- Synergies through overlapping partnership between PRACE and DEISA
- Enhancements and adaption where needed

Procurement strategy

- Analysis of European procurement procedures completed
  - Open
  - Restricted
  - Competitive dialogue
  - Negociated
  - Pre-commercial
- Work in progress
  - Definition of general procurement process
  - Definition of selection and evaluation criteria
  - Evaluation process for offers by vendors

PRACE web site

- The PRACE web presence with news, events, RSS feeds etc. http://www.prace-ri.eu
- Public deliverables
- Training material
- Special presentations
- http://www.prace-project.eu
- http://www.prace-project.eu/documents
- http://www.prace-project.eu/hpc-training
- http://www.prace-project.eu/hpc-training/prace-code-porting-videos

The PRACE website, www.prace-project.eu

Public deliverables available:http://www.prace-project.eu/documents

- D2.1.1 Report on options for a legal entity (pdf)
- D2.2.1 Report on analysis of adequate governance structure (pdf)
- D2.4.1 Initial report peer review process (pdf)
- D2.5.1 Analysis of HPC Ecosystem (pdf)
- D2.5.2 Report on Links with HPC Ecosystem (pdf)
- D2.6.1 Operational model analysis and initial specifications (pdf)
- . D3.1.6 Proceedings of first scientific conference (pdf)
- D3.2.1 First industrial seminar (pdf)
- D3.3.1 Survey of HPC education and training needs (pdf)
- D3.3.2 PRACE Summer School (pdf)
- D6.1 Identification and categorisation of applications and initial benchmarks suite (pdf)
- D6.2.2 Final report on application requirements (pdf)
- D6.3.1 Report on available performance analysis and benchmark tools, representative Benchmark (pdf)
- D7.2 Systems compliant with user requirements (pdf)
- D7.5.1 Technical requirement for the first Petaflop/s system(s) in 2009/2010 (pdf)
- D7.6.1 Procurement strategy (pdf)

Video training material already on web site

- Material from 4 workshops
- 48 hours video material

Thank you on behalf of the European Heavy Computing Community!

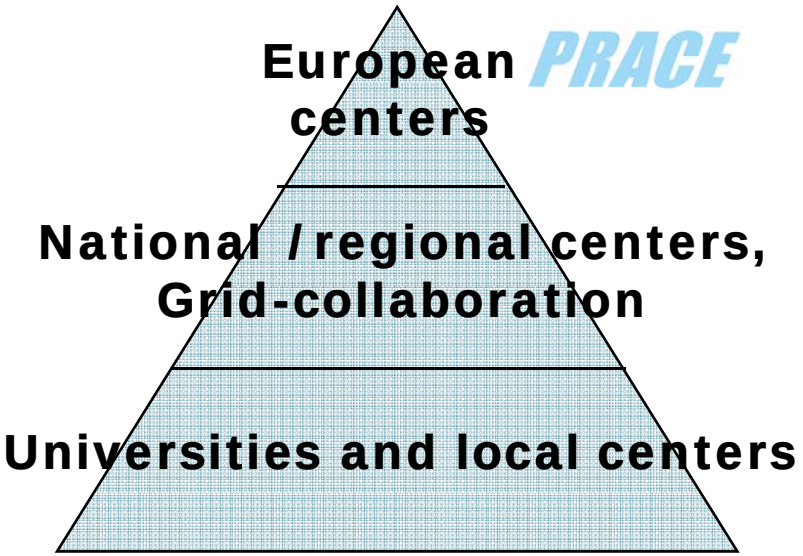
CSC (and Nordic) view and impact

Topics to consider

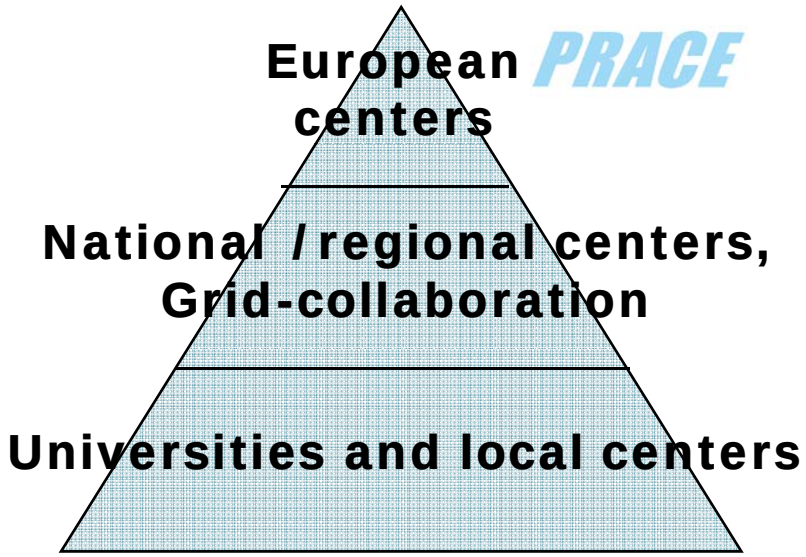
- Installing of Tier-0 or accessing it?
  - Number of scientists with ability to use +100000 cores in parallel?
  - Investment vs. benefits?
  - Possibilities to get access, if not in own control?
  - Competitive position if resources not available (with short notice)?
- Position of Nordic countries
  - Potential for ‘virtual Tier-0’, but where to place it and is it really needed?
  - Joining forces for applications, training, competence building etc.
  - Raise of the eco-efficient ICT: all the datacenters to the cool climate and green energy?

Some challenges with PRACE

- What is the cost to use Tier-0?
  - 'Donation only' is not sustainable
  - Paying is more difficult than in-kind
  - What kind of in-kind is accepted?
  - Will the "market" work?
- Integration of different Tiers
  - How to link Tier0 – Tier1?
  - What are the links to Tier2?
  - Is the Tiers at all a relevant abstraction?
    - Users could not care less in what Tier they are working - only interest to get the work done
- Relations between scientists (users) and PRACE centers
  - Need to speak the same language

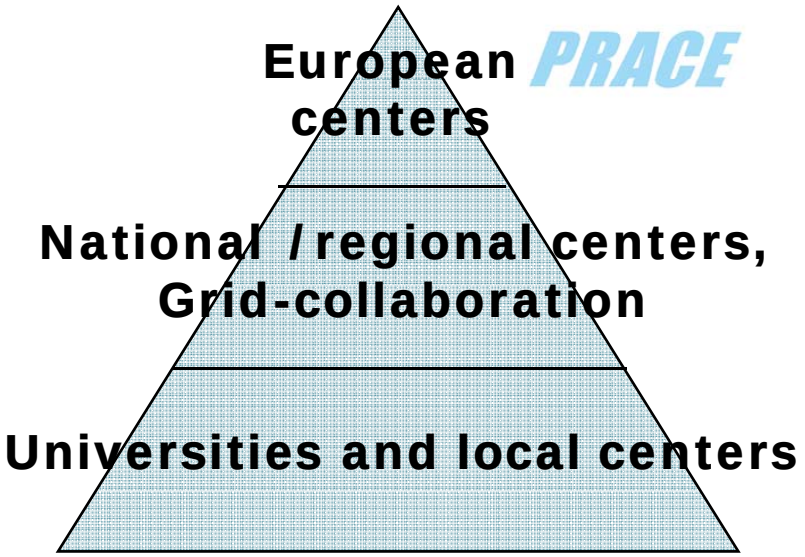


More issues…



1. How to guarantee access to the top of the pyramid for selected groups?
2. How to ensure there are competent users which can use the high end resources?
3. How to involve all countries who can contribute?
4. How to develop competence in home ground?
5. How to boost collaboration between research and e-infrastructure providers?
6. What are the principles of resource exchange (in-kind)?

How to benefit from the opportunity in Nordics



- National infrastructure close enough to the top
  - Stepping stone for code development
  - Ability to use high-end (hard to jump from laptop to 100000 cores)
  - Potential for resource exchange Tier1-Tier2
- Focus on application development, balanced e-infrastructure and competence development
- Nordic collaboration

Some conclusions

- PRACE is a unique opportunity, but it still needs a lot of work in shaping the offering
- Considerable development has been achieved since the first HPCEUR project back in 2004
  - Working with the full HPC Ecosystem instead of just peak performance hardware
- “Non-hosting” countries should be active and focus on their strengths, this way we can have impact